



Matrix representation of a Neural Network

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Matrix representation of a Neural Network

by
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June 2003

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1 Introduction

This paper describes the implementation of a three-layer feedforward backpropagation neural network.

The paper does not explain *feedforward*, *backpropagation* or what a *neural network* is. It is assumed, that the reader knows all this. If not please read chapters 2, 8 and 9 in *Parallel Distributed Processing*, by David Rumelhart (*Rumelhart 1986*) for an easy-to-read introduction.

What the paper does explain is how a *matrix representation* of a neural net allows for a very simple implementation.

The matrix representation is introduced in (*Rumelhart 1986, chapter 9*), but only for a two-layer linear network and the feedforward algorithm. This paper develops the idea further to three-layer non-linear networks and the backpropagation algorithm.

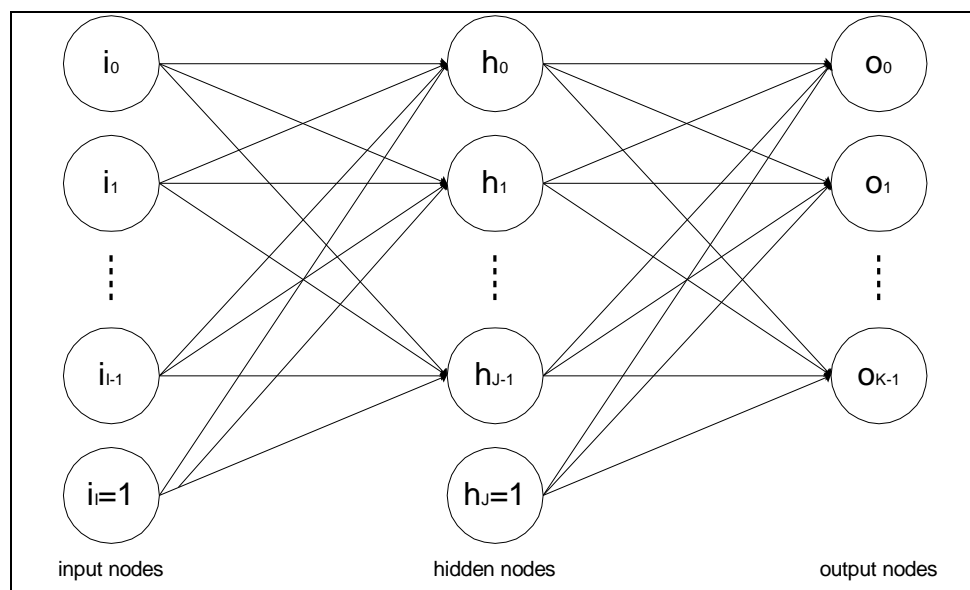


Figure 1

Figure 1 shows the layout of a three-layer network. There are I input nodes, J hidden nodes and K output nodes all indexed from 0. Bias-node for the hidden nodes is called i_I , and bias-node for the output nodes is called h_J .

2 The Weight Matrix

In the matrix representation the input, hidden and output nodes are represented by three vectors \mathbf{i} , \mathbf{h} and \mathbf{o} respectively. The weights connecting each layer are represented by a matrix. \mathbf{V} connects the input layer with the hidden layer, and \mathbf{W} connects the hidden layer with the output layer. See Figure 2.

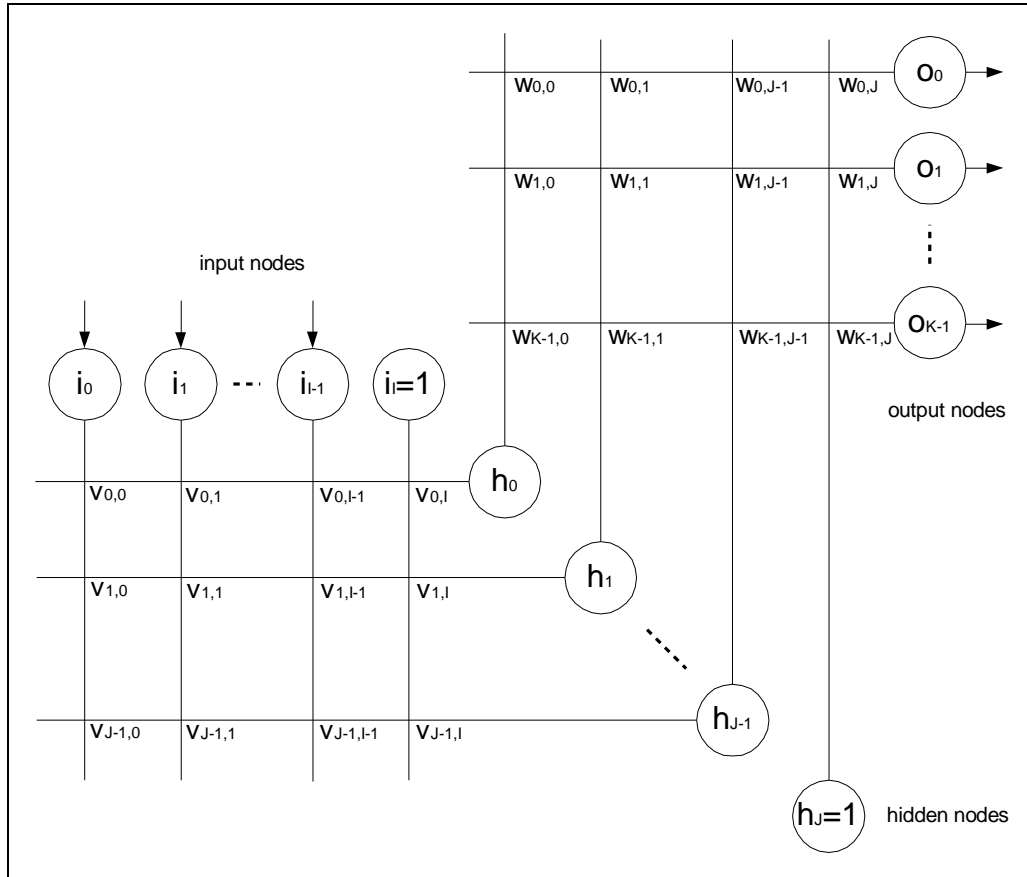


Figure 2

Definitions:

\mathbf{i} - input nodes vector,	dimension = l ,	indexed by $i \in [0, l-1]$
\mathbf{h} - hidden nodes vector,	dimension = J ,	indexed by $j \in [0, J-1]$
\mathbf{o} - output nodes vector,	dimension = K ,	indexed by $k \in [0, K-1]$
\mathbf{ib} - input nodes vector incl bias,	dimension = $l+1$,	indexed by $i \in [0, l]$
\mathbf{hb} - hidden nodes vector incl bias,	dimension = $J+1$,	indexed by $j \in [0, J]$
\mathbf{V} - weight matrix from \mathbf{ib} to \mathbf{h} ,	dimension = $J \times (l+1)$,	$V_{j,i}$ weight $\mathbf{ib}_i \rightarrow \mathbf{h}_j$
\mathbf{W} - weight matrix from \mathbf{hb} to \mathbf{o} ,	dimension = $K \times (J+1)$,	$W_{k,j}$ weight $\mathbf{hb}_j \rightarrow \mathbf{o}_k$

Bold denotes a vector or a matrix in the text.

2.1 Feedforward

The feedforward algorithm produces an output vector given an input vector. As described in (*Callan 1999, chapter 1*), the input to hidden node h_j is

$$\text{net}_j = V_{j,1} + \sum_{i=0}^{I-1} i_i V_{ji} \quad (1)$$

The naming convention of Callan is changed to match the definitions in this paper which follows (*Rummelhart 1986*). Note that Callan has interchanged the indices in the weight matrix.

The value of hidden node h_j is

$$\mathbf{h}_j = f(\text{net}_j) \quad (2)$$

Where $f()$ is the activation function defined as

$$f(x) = \frac{1}{1 + e^{-x}} \quad (3)$$

Using matrix-vector multiplication, the value of all hidden nodes \mathbf{h} can be calculated in a single operation

$$\mathbf{h} = F(\mathbf{V} \cdot \mathbf{ib}) \quad (4)$$

Where $F()$ is the vector function that takes $f()$ on all elements of it's argument.

Similarly the output vector is calculated from

$$\mathbf{o} = F(\mathbf{W} \cdot \mathbf{hb}) \quad (5)$$

\mathbf{ib} and \mathbf{hb} are produced from

$$\mathbf{ib}_i = i_i \text{ for } i \in [0..I-1], \quad \mathbf{ib}_I = 1 \quad (6)$$

$$\mathbf{hb}_j = h_j \text{ for } j \in [0..J-1], \quad \mathbf{hb}_J = 1 \quad (7)$$

2.2 Backpropagation

The backpropagation algorithm calculates the changes of the weights based on the error between the output \mathbf{o} as calculated the by the feedforward algorithm, and the desired target output value \mathbf{t} .

Definition:

\mathbf{t} - target vector,	dimension = K ,	indexed by $k \in [0, K-1]$
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From equation 11 in (*Rumelhart 1986, chapter 8*), we have the change of each weight:

$$\Delta W_{kj} = \eta \delta_k h_j \quad (8)$$

Where η is the *learning rate*, δ_k is the *error signal* form output node o_k , and h_j is the value of node h_j . This formula applies to all weights in the network. The error signal from the output layer and the hidden layer are calculated differently. Rumelhart defines the error signal as follows

$$\text{Error signal from output node } k \quad \delta o_k = o_k(1 - o_k)(t_k - o_k) \quad (9)$$

$$\text{Error signal from hidden node } j \quad \delta h_j = h_j(1 - h_j) \sum_{k=0}^{K-1} \delta o_k W_{kj} \quad (10)$$

Definition:

$\delta \mathbf{o}$ - error signal from output nodes	dimension = K ,	indexed by $k \in [0, K-1]$
$\delta \mathbf{h}$ - error signal from hidden nodes	dimension = J ,	indexed by $j \in [0, J-1]$

Now we are ready to calculate the weight change $\Delta \mathbf{W}$ for all weights in a single operation:

$$\begin{aligned} \Delta \mathbf{W} &= \eta \begin{bmatrix} \Delta W_{0,0} & \Delta W_{0,1} & \Delta W_{0,J-1} & \Delta W_{0,J} \\ \Delta W_{1,0} & \Delta W_{1,1} & \Delta W_{1,J-1} & \Delta W_{1,J} \\ \Delta W_{K-1,0} & \Delta W_{K-1,1} & \Delta W_{K-1,J-1} & \Delta W_{K-1,J} \end{bmatrix} \quad (11) \\ &= \eta \begin{bmatrix} \delta o_0 h_0 & \delta o_0 h_1 & \delta o_0 h_{J-1} & \delta o_0 h_J \\ \delta o_1 h_0 & \delta o_1 h_1 & \delta o_1 h_{J-1} & \delta o_1 h_J \\ \delta o_{K-1} h_0 & \delta o_{K-1} h_1 & \delta o_{K-1} h_{J-1} & \delta o_{K-1} h_J \end{bmatrix} \\ &= \eta \begin{bmatrix} \delta o_0 \\ \delta o_1 \\ \delta o_{K-1} \end{bmatrix} \otimes \begin{bmatrix} h_0 & h_1 & h_{J-1} & h_J \end{bmatrix} \\ &= \eta \cdot \delta \mathbf{o} \otimes \mathbf{h} \mathbf{b} \end{aligned}$$

So $\Delta \mathbf{W}$ is η times the outer product of $\delta \mathbf{o}$ and $\mathbf{h} \mathbf{b}$. \otimes is the operator for the outer product. Similarly for $\Delta \mathbf{V}$ we get

$$\Delta \mathbf{V} = \eta \cdot \delta \mathbf{h} \times \mathbf{i} \mathbf{b} \quad (12)$$

We need to express $\delta \mathbf{o}$ and $\delta \mathbf{h}$ in vector form. Let us define a vector multiplication operator $\%$ that multiplies the components of vector \mathbf{X} and \mathbf{Y} as follows:

$$\mathbf{X} \% \mathbf{Y} = \begin{bmatrix} X_1 * Y_1 \\ X_2 * Y_2 \\ \vdots \\ X_n * Y_n \end{bmatrix} \quad (13)$$

Calculating $\delta \mathbf{o}$ is easy:

$$\delta \mathbf{o} = \mathbf{o} \% (\mathbf{1} - \mathbf{o}) \% (\mathbf{t} - \mathbf{o}) \quad (14)$$

Where $\mathbf{1}$ is a vector of 1's with same dimension as \mathbf{o} .

Calculating $\delta \mathbf{h}$ requires a little more work. Let us define a vector \mathbf{s} as:

$$\mathbf{s} = \mathbf{W}^T \cdot \delta \mathbf{o} \quad (15)$$

\mathbf{W}^T is the transpose of \mathbf{W} . Expanding \mathbf{W} and $\delta \mathbf{o}$ gives us:

$$\begin{aligned} \mathbf{s} &= \begin{bmatrix} W_{0,0} & W_{0,1} & \dots & W_{0,J-1} & W_{0,J} \\ W_{1,0} & W_{1,1} & \dots & W_{1,J-1} & W_{1,J} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ W_{K-1,0} & W_{K-1,1} & \dots & W_{K-1,J-1} & W_{K-1,J} \end{bmatrix}^T \cdot \begin{bmatrix} \delta o_0 \\ \delta o_1 \\ \vdots \\ \delta o_{K-1} \end{bmatrix} \quad (16) \\ &= \begin{bmatrix} W_{0,0} & W_{0,1} & \dots & W_{K-1,0} \\ W_{0,1} & W_{0,2} & \dots & W_{K-1,1} \\ \vdots & \vdots & \ddots & \vdots \\ W_{0,J-1} & W_{0,J} & \dots & W_{K-1,J-1} \\ W_{1,0} & W_{1,1} & \dots & W_{K-1,J} \end{bmatrix} \cdot \begin{bmatrix} \delta o_0 \\ \delta o_1 \\ \vdots \\ \delta o_{K-1} \end{bmatrix} \\ &= \begin{bmatrix} \delta o_0 W_{0,0} & + \delta o_1 W_{1,0} & + \dots + \delta o_{K-1} W_{K-1,0} \\ \delta o_0 W_{0,1} & + \delta o_1 W_{1,1} & + \dots + \delta o_{K-1} W_{K-1,1} \\ \vdots & \vdots & \ddots & \vdots \\ \delta o_0 W_{0,J-1} & + \delta o_1 W_{1,J-1} & + \dots + \delta o_{K-1} W_{K-1,J-1} \\ \delta o_0 W_{0,J} & + \delta o_1 W_{1,J} & + \dots + \delta o_{K-1} W_{K-1,J} \end{bmatrix} \\ &= \begin{bmatrix} s_0 \\ s_1 \\ \vdots \\ s_{J-1} \\ s_J \end{bmatrix} \quad \text{where } s_j = \sum_{k=0}^{K-1} \delta o_k W_{kj} \end{aligned}$$

The component s_j is operand in the error signal δh_j . Note that we do not need an error signal from h_J since it is a bias node. Therefore we skip the last component of \mathbf{s} , and create a vector \mathbf{s} defined as:

$$s_j = s_j \text{ for } j \in [0..J-1] \quad (17)$$

Dimension of \mathbf{s} is J . Finally we can write $\delta \mathbf{h}$ as:

$$\delta \mathbf{h} = \mathbf{h} \% (\mathbf{1} - \mathbf{h}) \% \mathbf{s} \quad (18)$$

Here $\mathbf{1}$ has same dimension as \mathbf{h} .

Let us sum up the important equations of the backpropagation algorithm:

$$\text{Error signal from output nodes} \quad \delta \mathbf{o} = \mathbf{o} \% (\mathbf{1} - \mathbf{o}) \% (\mathbf{t} - \mathbf{o}) \quad (19)$$

$$\text{Changes of weights connected to output nodes} \quad \Delta \mathbf{W} = \eta \cdot \delta \mathbf{o} \times \mathbf{h} \mathbf{b} \quad (20)$$

$$\text{Propagated errors from output nodes} \quad \mathbf{s} = \mathbf{W}^T \cdot \delta \mathbf{o} \quad (21)$$

$$\text{Error signal from hidden nodes} \quad \delta \mathbf{h} = \mathbf{h} \% (\mathbf{1} - \mathbf{h}) \% \mathbf{s} \quad (22)$$

$$\text{Changes of weights connected to hidden nodes} \quad \Delta \mathbf{V} = \eta \cdot \delta \mathbf{h} \times \mathbf{i} \mathbf{b} \quad (23)$$

2.3 Squared Error

The squared error is a measure of the correctness of the network. It is calculated for each input pattern p . Rummelhart defines the squared error as:

$$E_p = \frac{1}{2} \sum_{k=0}^{K-1} (t_k - o_k)^2 \quad (24)$$

In vector notation using the inner product this is

$$E_p = \frac{1}{2} (\mathbf{t} - \mathbf{o}) \cdot (\mathbf{t} - \mathbf{o}) \quad (25)$$

Summing the squared errors for all patterns, we get the squared error E for an epoch

$$E = \sum_{p=1}^n E_p \quad (26)$$

Where n is the number of patterns in the training set.

3 References

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